TSRC TDDFT Summer School and Excited States Workshop

July 11-21, 2017, in Telluride, Colorado

School Organizers: Christine Isborn, Neepa Maitra, and Andre Schleife

Workshop Organizers: Christine Isborn, Neepa Maitra, Andre Schleife, and Xiaosong Li

Overview

The first US-based summer school and workshop on Time-Dependent Density Functional Theory (TDDFT) was held July 11-21, 2017 in Telluride, CO. TDDFT is increasingly used in computational molecular and materials science to calculate electronic-excitation spectra and dynamics in a wide variety of applications, including photocatalysis, photo-controlled bond dissociation, and light-induced charge transfer. Software development in this community targets multiple software packages, many of which are open source, such as octopus, NWchem and Qb@ll, which are the ones our school focused on. The goal of this first iteration was to create a home for a national community of scholars, including users and developers, with a deep understanding of TDDFT, its capabilities, limitations, and high-performance computing context. We used this opportunity to explore interest in such an event in the future and based on overwhelmingly positive feedback from students and teachers, we intend to hold a similar school+workshop every two years in the US, in order to maintain the high level of interest that we witnessed and the enthusiasm amongst participants.

Summary of School and Workshop Activities

The school consisted of theory lectures in the morning followed by hands-on practical sessions in the afternoon.

The morning lectures were 50 min each, with 20 minutes for questions and discussion. This was a successful format because it turned out to be highly interactive, with many questions by the students. Topics covered were: Fundamentals of DFT, Fundamentals of TDDFT, Linear Response, Excitations in Solution, Excitations in the Solid-State, Charge-Transfer and Optimally-Tuned Hybrids, Real-Time TDDFT, time-dependent current DFT, and Non-Adiabatic Electron-Ion Dynamics. All lecturers uploaded their materials to a web site that all students were able to access. Each instructor (Kieron Burke, Mark Casida, Christine Isborn, Neepa Maitra, Shane Parker, Lucia Reining, Andre Schleife) gave two lectures.

The first two afternoon hands-on sessions, led by Niri Govind and Ken Lopata, focused on the NWChem code, but also used python, octave, and gnuplot. Students learned how to set up an input file to calculate excitation energies using linear response TDDFT and also perform electron dynamics using real-time TDDFT. All students were able to have a working code for modeling charge-transfer excitations with different functionals and peak-transfer from resonant laser-induced excitation. The second two afternoon sessions, led by Alberto Castro and Xavier Andrade, focussed on the Qb@ll and Octopus codes, in order to complement the local-orbital aspect of the first two sessions with the plane-wave approach to describe Kohn-Sham states. Students applied a laser field to a molecule and analyzed the resulting electron dynamics,

performed Ehrenfest dynamics to model photodissociation, and simulated a high harmonic generation spectrum. All hands-on sessions were run on NERSC supercomputers, in order to provide students with a "real-world" experience of how to run simulations in a high-performance-computing context. To this end, we successfully applied for and used NERSC training accounts.

On the final day all instructors were present for a one-hour panel discussion with the students. This discussion was remarkably lively; a large fraction of the students remained engaged with extremely pertinent questions throughout the discussion, on prospects of advances in theoretical functional development as well as practical application of the theory. The discussion even went over the scheduled hour, even after the full week of lectures and time for questions.

We held a poster session which enabled students to directly discuss their on-going work with the lecturers and with other students. The breakfasts, lunches, and dinners provided further opportunity for discussion. In particular, the breakfasts, being provided by TSRC on-site, allowed many participants to interact and get to know each other. For the workshop, lunches were provided on-site, enabling extensive small-group discussions of the research presented in the workshop talks and effectively connecting the students who stayed for the workshop with the workshop speakers.

The workshop topics spanned recent developments and applications in TDDFT, from molecules to solids, and from linear response to strong fields. The overall salient observation was the extensive range of applications of TDDFT to quite complex situations, and the depth of the analysis, both in terms of the computational efficiency as well as functional accuracy. For example, with electron scattering, we heard talks on dynamical features in the exact time-dependent exchange-correlation potential in electron-molecule scattering, and, at the other extreme, results on scattering in warm dense plasmas. The advances in stopping power calculations over the recent years was notable for the size and scope of what is possible today; when is it important to include the vibrations of the lattice and when can they be ignored, when must we go beyond the pseudopotential approximation, and what is the effect of defects in semiconductors on stopping power. Then again on the more fundamental side, there was a talk on whether a long-time thermal equilibrium for TDDFT can be defined. Effects arising from quantized radiation fields coupled to molecules were discussed, with new density-functional methods that bridge quantum optics with quantum chemistry, and recent advances in multiscale methods for strong classical fields coupled to electron-ion dynamics in materials were presented. New developments of TDDFT in solvents were presented, in particular careful examination of the effects of coupling explicit quantum solvent with a polarizable continuum. The full range of talks and topics is evident in the talk titles presented below. One afternoon session was devoted to talks in honor of Giovanni Vignale's 60th birthday. Applications of TDDFT to such complex situations, together with analysis of the fundamental aspects, beyond a simple calculation of spectra of intermediate-size molecules or periodic solids, exemplifies the progress in the field in recent years.

Participants of School and Workshop

The TDDFT school drew about 60 applicants from around the world, out of whom we selected 33 based on their promise for a career in science and their research field of interest. We strove for a balance of students from large and small institutions, from groups with established and early-career research advisors, and from a range of experience levels. Of the 33 students, 8 were women.

Student Participants, Summer School:

1. Cheng-Wei Lee, University of Illinois at Urbana-Champaign
2. Niraj Nepal, Temple University
3. Christopher Myers, University at Albany
4. Ravithree Senanayake, Kansas State University
5. John Philbin, UC Berkeley
6. Guo Chen, UC Irvine
7. Daniel Burrill, University of Pittsburgh
8. Edwin Quashie, Lawrence Livermore National Laboratory
9. Nathan Koocher, Northwestern University
10. Zuxin Jin, University of Pennsylvania
11. Ying Zhu, Ohio State University
12. Adam Bruner, Lousiana State University
13. Francisca Sagredo, University of California Irvine
14. Hemanadhan Myneni, University of Delaware
15. Sudheer Peddathimmareddy, Rutgers University
16. Dominik Maximilian Juraschek, ETH Zurich, Switzerland
17. Alexander Kohn, MIT
18. Imon Mandal, Tata Institute of Fundamental Research (TIFR), Mumbai
19. Dillon Yost, Univ. North Carolina, Chapel Hill
20. Rodrigo Freitas, UC Berkeley
21. Irene Metz, University of Iowa
22. Jon Bender, UT Austin
23. Andrew Sifain, Los Alamos National Laboratory
24. Amelia Fitzsimmons, Oak Ridge National Laboratory
25. Arthur De Vos, Ghent University
26. Feng Wu, UC Santa Cruz
27. Jane Herriman, Caltech
28. Yanal Oueis, Purdue University
29. Graeme Gossel, Hunter College
30. Jacob Wilmer, UC Merced
31. Edward Pluhar, University of Missouri
32. Aliya Mukazhanova, Boston University
33. Matthew Anderson, University of Missouri

The Excited States workshop had 34 speakers. Some of the speakers were students from the summer school that remained for the workshop. The talks spanned many research areas, and the titles are given below.

Excited States Workshop Participants, Affiliations, and Talk Titles:

1. Kieron Burke, Dept of Chemistry, UC Irvine: *Excitation energies from ensemble DFT*
2. Yasumitsu Suzuki, Dept of Physics, Tokyo University of Science: *Exact time-dependent exchange-correlation potentials in electron scattering processes*
3. Prineha Narang, Materials Science, Harvard University: *Excited state and Quantum-engineered Materials*
4. Graeme Gossel, Dept. of Physics and Astronomy, Hunter College CUNY : *Exact factorization of the electron-nuclear wavefunction: properties, approximations, and applications*
5. Giovanni Vignale, Dept of Physics and Astronomy, University of Missouri: *Berry curvature and excited states at the boundary of an electron liquid*
6. Carsten Ullrich, Dept of Physics and Astronomy, University of Missouri: *Spin waves in chiral two-dimensional electron systems*
7. Florian Eich, Max-Planck Institute Hamburg: *Charge and Energy Transport at the Nanoscale: A Density Functional Perspective*
8. Irene D'Amico, Dept of Physics, York University, UK: *Using DFT concepts and tools for quantum thermodynamics*
9. Christine Isborn, Dept of Chemistry, U.C. Merced: *Excited States in Solution: Towards More Accurate Absorption Spectra*
10. Matthieu Verstraete, Dept of Physics, University of Liege, Belgium: *Long-range dispersion forces between molecules subject to attosecond pulses from ab initio calculations*
11. Imon Mandal, Tata Institute of Fundamental Research (TIFR), Mumbai: *Photoinduced Charge Transfer transitions Associated with Charged Amino Acids:TDDFT Reveals a new Spectral Marker for Proteins*
12. Andrew Baczewski, Center for Computing Research, Sandia National Laboratory: *Warm Dense Matter: Opportunities and challenges for TDDFT*
13. André Schleife, Dept of Materials Science and Engineering, University of Illinois at Urbana-Champaign: *Excited-electron dynamics near surfaces: Particle radiation in real-time TDDFT*
14. Xavier Andrade-Valencia, Lawrence Livermore National Laboratory: *Non-linear effects in conductivity*
15. John Parkhill, Dept. of Chemistry, University of Notre Dame: *Pumping and Relaxation in TDDFT: Patches and problems*
16. David Strubbe, Dept. of Physics, U.C. Merced: *Excited-state forces in TDDFT and the Bethe-Salpeter equation*
17. Heiko Appel, Max Planck Institute for Structure and Dynamics of Matter, Hamburg: *Ab-initio description of classical and quantized photon fields coupled to molecular systems*
18. Shane Parker, Dept. of Chemistry, U. C. Irvine: *Nonlinear properties from TDDFT: trials and tribulations, quadratic response theory*
19. Dominik Juraschek, ETH Zurich, Switzerland: *Dynamical Multiferroicity*
20. Mark Casida, Dept. of Chemistry, University of Grenoble, France: *On the calculation of Δ⟨S2⟩ for electronic excitations in TDDFT*

21. Xiaosong Li, Dept of Chemistry, University of Washington: *Two-Component Noncollinear Time-Dependent Density Functional Theory for Excited State Calculations*
22. Alberto Castro, Institute for Biocomputation and Physics of Complex Systems,University of Zaragoza, Spain: *Brief reports on (1) Control for quantum optics processes; and (2) Propagators for the time-dependent Kohn-Sham equations*
23. Yoshiyuki Miyamoto, National Institute of Advanced Industrial Science & Technology (AIST), Tsukuba, Japan: *Laser-field enhancement and coherent electron dynamics in low-dimensional materials examined by real-time TDDFT*
24. Dillon Yost, Univ. North Carolina, Chapel Hill: *Recent progress in modeling electronic stopping using non-equilibrium RT-TDDFT simulations*
25. Barry Dunietz, Dept of Chemistry, Kent State University: *First-principles based studies of photo-induced electron transfer and transport through molecular-resolved interfaces*
26. Michele Pavanello, Dept. of Chemistry, Rutgers-Newark: *Electronic properties of liquids and materials from subsystem and orbital-free DFT*
27. Lucia Reining, Ecole Polytechnique, Palaiseau, France: *Density functionals for the dynamic structure factor and more*
28. Kazuhiro Yabana, Center for Computational Sciences, University of Tsukuba: *Real-time TDDFT simulations for interactions of ultrashort laser pulses with solids, coupling to Maxwell's equations*
29. Norah Hoffmann, Max Planck Institute for Structure and Dynamics of Matter, Hamburg: *Ab-Initio Description of Photoinduced Processes Beyond Classical Maxwell Theory*
30. Simone Marocchi, Institute of Physics, University of Sao Paolo, Brazil: *Quantum mechanics in metric space: distances between exchange-only correlations*
31. Arindam Chakraborty, Dept of Chemistry, Syracuse University: *Linked-cluster formulation of screened electron-hole interaction from explicitly-correlated geminal functions without using unoccupied states*
32. Normand Modine, Center for Integrated Nanotechnologies, Sandia National Lab: *Long-time limit of TDDFT*
33. Cheng-Wei Lee, University of Illinois at Urbana Champaign: *Electron-Ion Dynamics in Semiconductors with defects under Ion Irradiation*
34. Neepa Maitra, Dept of Physics, Hunter College and Graduate Center CUNY: *New Approaches to Non-Adiabatic Functionals*

Of the 34 workshop speakers, 8 were students/post-docs (Gossel, Mandal, Parker, Marocchi, Lee, Hoffmann, Yost, Juraschek, Eich), 10 were early career faculty/scientists (Isborn, Narang, Schleife, Suzuki, Eich, Pavanello, Strubbe, Andrade-Valencia, Parkhill, Baczewski), and 7 were women (Mandal, Hoffmann, Maitra, Isborn, Reining, D'Amico, Narang).

Telluride Science Research Center Summer School on Time-Dependent Density Functional Theory

July 11-15, 2017

- Location: Telluride Intermediate School, 725 West Colorado Avenue

- Talks will be 50 minutes plus 15 minutes for questions and discussion
- Practical sessions will be 3.5 hours
- A twenty-minute coffee break is scheduled for both morning and afternoon sessions
- iCal/Google Calendar/Outlook compatible schedule: https://goo.gl/dB8fZJ

- Any questions about the schedule should be directed to school organizers: Christine Isborn (cisborn@ucmerced.edu), Neepa Maitra (nmaitra@hunter.cuny.edu), or Andre Schleife (schleife@illinois.edu)

- Any questions about logistics should be directed to TSRC executive director Mark Kozak (mark@telluridescience.org) 970-708-4426, or to Kristen Redd (kristen@telluridescience.org), 970-708-0827, for lodging questions.

- **TSRC Town Talk on Tuesday, July 11th**, 6-7:15 pm, Conference Center in Mountain Village: Town Talk, “Water: Separating Science from Pseudoscience”, Kenneth D. Jordan, U. Pittsburgh.

- **Picnic on Thursday, July 13th,** 6-8 pm, under the tent at the Elementary School (family and guests welcome free of charge)

- **Poster Session on Friday, July 14th,** 6-9 pm, under the tent at the Elementary School (light drinks provided)

- Breakfast Tuesday-Friday is included in the registration cost and will be provided at TSRC from 8:00 – 8:30 am

- Lunch **on Tuesday** will be a working lunch, **provided** at TSRC, to ensure computers are ready for the afternoon sessions. **You are responsible for your own for lunch Weds-Sat.**

	8:00 – 8:30 AM	MORNING 8:30 AM – 12:05 PM	12:05 – 2:00 PM	AFTERNOON 2:00 PM – 5:40 PM	EVENING
Tue July 11th	Breakfast at TSRC	TDDFT Fundamentals I & II *(Maitra)* Linear Response I *(Casida)*	Lunch at TSRC (Debug your virtual environment!)	NWChem *Govind, Lopata*	Town Talk, 6:00-7:15 PM (Conference Center in Mountain Village)
Weds July 12th	Breakfast at TSRC	Linear Response II *(Casida)* Charge-transfer and opt-tuned hybrids *(Isborn)* Real-time TDDFT *(Schleife)*	Lunch on your own	NWChem *Govind, Lopata*	
Thurs July 13th	Breakfast at TSRC	Excited States in Solution *(Isborn)* Excitations in solid-state I & II *(Reining)*	Lunch on your own	Octopus & Qb@ll *Castro, Andrade*	TSRC Picnic, 6:00 – 8:00 PM (Under tent at Elementary School)
Fri July 14th	Breakfast at TSRC	DFT Fundamentals I & II *(Burke)* Non-adiabatic electron-ion dynamics I *(Parker)*	Lunch on your own	Octopus & Qb@ll *Castro, Andrade*	Poster Session (Under the tent at the Elementary School)
Sat July 15th	Breakfast at TSRC	Non-adiabatic electron-ion dynamics II *(Parker)* TDCDFT *(Schleife)* Panel: Open Problems and Perspectives *(All lecturers+ Vignale)*		Free	

Telluride Science Research Center Workshop
Excited States: Electronic Structure and Dynamics
July 17-21, 2017

- Location: Telluride Intermediate School, 725 West Colorado Avenue

- Invited talks will be 35 minutes plus 10 minutes for questions and discussion. Student & post-doc talks will be 15 minutes plus 5 minutes for questions and discussion.

- A twenty-minute coffee break is scheduled for both morning and afternoon sessions

- Any questions about the schedule should be directed to workshop organizers: Christine Isborn (cisborn@ucmerced.edu), Xiaosong Li (xsli@uw.edu), Neepa Maitra (nmaitra@hunter.cuny.edu), or Andre Schleife (schleife@illinois.edu)

- Any questions about logistics should be directed to TSRC executive director Mark Kozak (mark@telluridescience.org) 970-708-4426, or to Kristen Redd (kristen@telluridescience.org), 970-708-0827 for lodging questions.

- **TSRC Town Talk on Tuesday, July 18th**, 6-7:15 pm, Conference Center in Mountain Village: “New Materials For Solar Energy Capture and Conversion,” by Natalie Stingelin and Chad Risko

- **Picnic on Wednesday, July 19th,** 6-9 pm, under the tent at the school (family and guests welcome free of charge)

- Breakfast Monday-Friday is included in the registration cost and will be provided at TSRC from 8:30 – 9:00 am

- Lunch Monday-Thursday is included in the registration cost and will be provided at TSRC from 12:40 – 2:00 pm

	8:30 – 9:00 AM	MORNING 9:00 AM – 12:40 PM	12:40 – 2:00 PM	AFTERNOON 2:00 PM – 5:40 PM	EVENING
Mon July 17th	Breakfast at TSRC	Burke Suzuki ***Break*** *Gossel* Narang Crawford	Lunch at TSRC	Special Session for Giovanni Vignale ***Break*** Ullrich Eich D'Amico	Free
Tues July 18th	Breakfast at TSRC	Isborn Herbert ***Break*** *Mandal* Dunietz Baczewski	Lunch at TSRC	Schleife Andrade ***Break*** Parkhill Strubbe	Town Talk, 6:00-7:15 PM (Conference Center in Mountain Village)
Wed July 19th	Breakfast at TSRC	Free	Lunch at TSRC	Appel Parker ***Break*** *Juraschek* Casida Li	TSRC Picnic, 6:00 – 9:00 PM (Under the tent at the Elementary School)
Thurs July 20th	Breakfast at TSRC	Castro Miyamoto ***Break*** *Yost* Correa Pavanello	Lunch at TSRC	Reining Yabana ***Break*** *Hoffmann, Marocchi* Chakraborty	Free
Fri July 21st	Breakfast at TSRC	Maitra Modine ***Break*** *Lee* Verstraete			

- Invited talks (35 min + 10 min) are in regular font, student and post-doc talks (15 min + 5 min) are in *italic*

Monday, July 17th

8:30 AM – 9:00 AM. Breakfast at TSRC

9:00 AM – 9:45 AM. Kieron Burke:
Linear response TDDFT for the two-site Hubbard model
9:45 AM – 10:30 AM. Yasumitsu Suzuki:
Exact time-dependent exchange-correlation potentials in electron scattering processes
10:30 AM – 10:50 AM. Break
10:50 AM – 11:10 AM Graeme Gossel:
Ex*act factorization of the electron-nuclear, wavefunction: properties, approximations, and applications*
11:10 AM – 11:55 AM Prineha Narang:
Excited state and Quantum-engineered Materials
11:55 AM – 12:30 PM T. Daniel Crawford: *MolSSI*

12:40 PM – 1:30 PM. Lunch at TSRC

2:00 PM – 2:20 PM. Neepa Maitra:
Intro to session in honor of Giovanni Vignale's 60th birthday
2:20 PM – 3:20 PM. Giovanni Vignale:
Berry curvature and excited states at the boundary of an electron liquid
3**:20 PM – 3:50 PM. Break**
3:50 PM – 4:35 PM Carsten Ullrich:
Spin waves in chiral two-dimensional electron systems
4:35 PM – 5:20 PM Florian Eich:
Charge and Energy Transport at the Nanoscale: A Density Functional Perspective
5:20 PM – 6:05 PM Irene D'Amico:
Using DFT concepts and tools for quantum thermodynamics

Tuesday, July 18th

8:30 AM – 9:00 AM. Breakfast at TSRC

9:00 AM – 9:45 AM. Christine Isborn:
Excited States in Solution: Towards More Accurate Absorption Spectra
9:45 AM – 10:30 AM. John Herbert:
First-Principles Exciton Models
10:30 AM – 10:50 AM. Break
10:50 AM – 11:10 AM Imon Mandal:
Photoinduced Charge Transfer transitions Associated with Charged Amino Acids:TDDFT Reveals a new Spectral Marker for Proteins

11:10 AM – 11:55 AM Barry Dunietz:
First-principles based studies of photo-induced electron transfer and transport through molecular-resolved interfaces
11:55 AM – 12:40 PM Andrew Baczewski:
Warm Dense Matter: Opportunities and challenges for TDDFT

12:40 PM – 1:30 PM. Lunch at TSRC

2:00 PM – 2:45 PM. André Schleife:
Excited-electron dynamics near surfaces: Particle radiation in real-time TDDFT
2:45 PM – 3:30 PM. Xavier Andrade:
Non-linear conductivity of metals from real-time TDDFT
3:30 PM – 3:50 PM. Break
3:50 PM – 4:35 PM John Parkhill:
Pumping and Relaxation in TDDFT: Patches and problems
4:35 PM – 5:20 PM David Strubbe:
Excited-state forces in TDDFT and the Bethe-Salpeter equation

6:00 PM – 7:25 PM. Town Talk in Mountain Village. "New Materials For Solar Energy Capture and Conversion," by Natalie Stingelin and Chad Risko

Wednesday, July 19th

8:30 AM – 9:00 AM. Breakfast at TSRC
Free Time
12:40 PM – 1:30 PM. Lunch at TSRC

2:00 PM – 2:45 PM. Heiko Appel:
Ab-initio description of classical and quantized photon fields coupled to molecular systems
2:45 PM – 3:30 PM. Shane Parker:
Nonlinear properties from TDDFT: trials and tribulations, quadratic response theory
3:30 PM – 3:50 PM. Break
3:50 PM – 4:10 PM Dominik Juraschek:
Dynamical Multiferroicity
4:10 PM – 4:55 PM Mark Casida:
On the calculation of $\Delta\langle S^2\rangle$ for electronic excitations in TDDFT
4:55 PM – 5:40 PM Xiaosong Li:
Two-Component Noncollinear Time-Dependent Density Functional Theory for Excited State Calculations
6:00 PM – 9:00 PM. TSRC Picnic. Under the tent at the Elementary School

Thursday, July 20th

8:30 AM – 9:00 AM. Breakfast at TSRC

9:00 AM – 9:45 AM. Alberto Castro:
Brief reports on (1) Control for quantum optics processes; and (2) Propagators for the time-dependent Kohn-Sham equations
9:45 AM – 10:30 AM. Yoshiyuki Miyamoto:
Laser-field enhancement and coherent electron dynamics in low-dimensional materials examined by real-time TDDFT
10:30 AM – 10:50 AM. Break
10:50 AM – 11:10 AM Dillon Yost:
Recent progress in modeling electronic stopping using non-equilibrium RT-TDDFT simulations
11:10 AM – 11:55 AM Alfredo Correa:
Ab initio electron dynamics: from stopping power to the non-linear electrical conductivity of materials
11:55 AM – 12:40 PM Michele Pavanello:
Electronic properties of liquids and materials from subsystem and orbital-free DFT

12:40 PM – 1:30 PM. Lunch at TSRC

2:00 PM – 2:45 PM. Lucia Reining:
Density functionals for the dynamic structure factor and more
2:45 PM – 3:30 PM. Kazuhiro Yabana:
Real-time TDDFT simulations for interactions of ultrashort laser pulses with solids, coupling to Maxwell's equations
3:30 PM – 3:50 PM. Break
3:50 PM – 4:10 PM Norah Hoffmann:
Ab-Initio Description of Photoinduced Processes Beyond Classical Maxwell Theory
4:10 PM – 4:30 PM Simone Marocchi:
Quantum mechanics in metric space: distances between exchange-only correlations
4:30 PM – 5:15 PM Arindam Chakraborty:
Linked-cluster formulation of screened electron-hole interaction from explicitly-correlated geminal functions without using unoccupied states

Friday, July 21st

8:30 AM – 9:00 AM. Breakfast at TSRC

9:00 AM – 9:45 AM. Neepa Maitra:
New Approaches to Non-Adiabatic Functionals
9:45 AM – 10:30 AM. Normand Modine:
Long-time Behavior of Time-Dependent Density Functional Theory
10:30 AM – 10:50 AM. Break
10:50 AM – 11:10 AM Cheng-Wei Lee:
Electron-Ion Dynamics in Semiconductors with defects under Ion Irradiation
11:10 AM – 11:55 AM Matthieu Verstraete:
Long-range dispersion forces between molecules subject to attosecond pulses from ab initio calculations